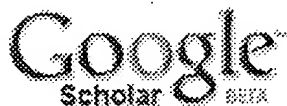


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S Hahn, G Stock - Chemical Physics, 2000 - theochem.uni-frankfurt.de

... Exact time-dependent wave-packet calculations have been reported including up to four **nuclear** degrees of freedom, showing that the model is suitable to ...

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T Kakitani, H Kakitani - Biophysics of Structure and Mechanism, 1979 - springerlink.com

... chromophore and opsin. At present, X-ray analysis of the three-dimensional structure of rhodopsin has not been successful. Studies so ...

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The Structure of Floppy Molecules: The Rg: XH/D (Rg= Ar, Ne, and Kr) Family of Complexes

CC Carter, HS Lee, AB McCoy, TA Miller - Dynamics - spectroscopy.mps.ohio-state.edu

... 43 we use J and j to represent the total angular momenta, excluding **nuclear** spin, of the complex and of the diatom fragment, respectively. (Here and throughout ...

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... Therefore another objective is the validation of the **spectroscopic model**, underlying the analysis ... weight factors g N , electronic ground state and **nuclear** spin I ...

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Spectra of cosmic X-ray sources

SS HOLT, R MCCRAY - Annual review of astronomy and astrophysics., 1982 - astro.annualreviews.org

... Because the coronal **spectroscopic model** should be appropriate to first order, the uncertainty in ... Models for X rays incident on a one-dimensional slab, used to ...

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Fe (II)/ α -Ketoglutarate-Dependent Hydroxylases and Related Enzymes

R Hausinger - Critical Reviews in Biochemistry and Molecular Biology, 2004 - dx.doi.org

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eIF-5A: eukaryotic initiation factor 5A; ENDOR: elec- tron **nuclear** double resonance ...

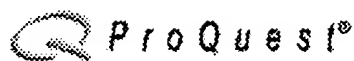
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"multi-dimensional" + "spectroscopic" + "model" + "heteronuclear"

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In this paper, we introduce self-tuning histograms. Although similar in structure to traditional histograms, these histograms infer data distributions not by examining the data or a sample thereof, but by using feedback from the query execution engine about the actual selectivity of range selection operators to progressively refine the histogram. Since the cost of building and maintaining self-tuning histograms is independent of the data size, self-tuning histograms provide a remarkably ine ...

4 Research track paper: A general model for clustering binary data



Tao Li

August 2005 **Proceeding of the eleventh ACM SIGKDD international conference on Knowledge discovery in data mining KDD '05**

Publisher: ACM Press

Full text available: [pdf\(628.85 KB\)](#) Additional Information: [full citation](#), [abstract](#), [references](#), [index terms](#)

Clustering is the problem of identifying the distribution of patterns and intrinsic correlations in large data sets by partitioning the data points into similarity classes. This paper studies the problem of clustering binary data. This is the case for market basket datasets where the transactions contain items and for document datasets where the documents contain "bag of words". The contribution of the paper is three-fold. First a general binary data clustering model is presented. The model trea ...

Keywords: binary data, clustering, general model, matrix approximation

5 Efficient co-triangulation of large data sets

Henrik Weimer, Joe Warren, Jane Troutner, Wendell Wiggins, John Shrout

October 1998 **Proceedings of the conference on Visualization '98**

Publisher: IEEE Computer Society Press

Full text available: [pdf\(1.41 MB\)](#) [Publisher Site](#) Additional Information: [full citation](#), [references](#), [index terms](#)

Keywords: Delaunay triangulation, computational geometry, data-structures, higher-dimensional approximation, multi-dimensional approximation, scattered data

6 A review of vessel extraction techniques and algorithms



Cemil Kirbas, Francis Quek

June 2004 **ACM Computing Surveys (CSUR)**, Volume 36 Issue 2

Publisher: ACM Press

Full text available: [pdf\(8.06 MB\)](#) Additional Information: [full citation](#), [abstract](#), [references](#), [index terms](#)

Vessel segmentation algorithms are the critical components of circulatory blood vessel analysis systems. We present a survey of vessel extraction techniques and algorithms. We put the various vessel extraction approaches and techniques in perspective by means of a classification of the existing research. While we have mainly targeted the extraction of blood vessels, neurovascular structure in particular, we have also reviewed some of the segmentation methods for the tubular objects that show ...

Keywords: Magnetic resonance angiography, X-ray angiography, medical imaging, neurovascular, vessel extraction

7 Reports from related meetings: Interface '99: a data mining overview

Arnold Goodman

 January 2000 **ACM SIGKDD Explorations Newsletter**, Volume 1 Issue 2


Publisher: ACM Press

Full text available:  [pdf\(851.62 KB\)](#) Additional Information: [full citation](#), [abstract](#), [references](#)

This personal overview of Interface '99 is intended to communicate its meaning and relevance to SIGKDD, as well as provide valuable information on trends within the Interface for data miners seeking to learn more about statistics. In addition, it is the newest link in a bridge between the Interface and KDD begun by References 2-4 and the sessions on KDD at Interface '98 and Interface '99.


Keywords: review of Interface'99 conference, statistics

8 [SCAAT: incremental tracking with incomplete information](#) 

 Greg Welch, Gary Bishop


August 1997 **Proceedings of the 24th annual conference on Computer graphics and interactive techniques**

Publisher: ACM Press/Addison-Wesley Publishing Co.

Full text available:  [pdf\(104.69 KB\)](#) Additional Information: [full citation](#), [references](#), [citations](#), [index terms](#)


Keywords: Kalman filter, autocalibration, calibration, delay, feature tracking, latency, sensor fusion, virtual environments tracking

9 [Statistical profile estimation in database systems](#) 

 Michael V. Mannino, Paicheng Chu, Thomas Sager

September 1988 **ACM Computing Surveys (CSUR)**, Volume 20 Issue 3

Publisher: ACM Press

Full text available:  [pdf\(2.94 MB\)](#) Additional Information: [full citation](#), [abstract](#), [references](#), [citations](#), [index terms](#)


A statistical profile summarizes the instances of a database. It describes aspects such as the number of tuples, the number of values, the distribution of values, the correlation between value sets, and the distribution of tuples among secondary storage units. Estimation of database profiles is critical in the problems of query optimization, physical database design, and database performance prediction. This paper describes a model of a database of profile, relates this model to estimating ...

10 [Special issue on independent components analysis: Blind separation of post-nonlinear mixtures using linearizing transformations and temporal decorrelation](#) 

Andreas Ziehe, Motoaki Kawanabe, Stefan Harmeling, Klaus-Robert Müller

December 2003 **The Journal of Machine Learning Research**, Volume 4

Publisher: MIT Press

Full text available:  [pdf\(3.39 MB\)](#) Additional Information: [full citation](#), [abstract](#), [index terms](#)

We propose two methods that reduce the post-nonlinear blind source separation problem (PNL-BSS) to a linear BSS problem. The first method is based on the concept of *maximal correlation*: we apply the alternating conditional expectation (ACE) algorithm---a powerful technique from non-parametric statistics---to approximately invert the componentwise non-linear functions. The second method is a Gaussianizing transformation, which is motivated by the fact that linearly mixed signals bef ...

11 [Research papers: estimation and approximation: Relational confidence bounds are easy with the bootstrap](#) 



Abhijit Pol, Christopher Jermaine

June 2005 **Proceedings of the 2005 ACM SIGMOD international conference on Management of data**

Publisher: ACM Press

Full text available: [pdf\(337.51 KB\)](#) Additional Information: [full citation](#), [abstract](#), [references](#)

Statistical estimation and approximate query processing have become increasingly prevalent applications for database systems. However, approximation is usually of little use without some sort of guarantee on estimation accuracy, or "confidence bound." Analytically deriving probabilistic guarantees for database queries over sampled data is a daunting task, not suitable for the faint of heart, and certainly beyond the expertise of the typical database system end-user. This paper considers the prob ...

12 Designing and mining multi-terabyte astronomy archives: the Sloan Digital Sky



Survey

Alexander S. Szalay, Peter Z. Kunszt, Ani Thakar, Jim Gray, Don Slutz, Robert J. Brunner
May 2000 **ACM SIGMOD Record , Proceedings of the 2000 ACM SIGMOD international conference on Management of data SIGMOD '00**, Volume 29 Issue 2

Publisher: ACM Press

Full text available: [pdf\(429.09 KB\)](#) Additional Information: [full citation](#), [abstract](#), [references](#), [citations](#), [index terms](#)

The next-generation astronomy digital archives will cover most of the sky at fine resolution in many wavelengths, from X-rays, through ultraviolet, optical, and infrared. The archives will be stored at diverse geographical locations. One of the first of these projects, the Sloan Digital Sky Survey (SDSS) is creating a 5-wavelength catalog over 10,000 square degrees of the sky (see <http://www.sdss.org/>). The 200 million objects in the multi-terabyte database will have mostly numerical attribut ...

Keywords: Internet, archive, astronomy, data analysis, data mining, database, scalable

13 Compression Domain Volume Rendering



Jens Schneider, Rudiger Westermann

October 2003 **Proceedings of the 14th IEEE Visualization 2003 (VIS'03) VIS '03**

Publisher: IEEE Computer Society

Full text available: [pdf\(1.23 MB\)](#) Additional Information: [full citation](#), [abstract](#)

A survey of graphics developers on the issue of texture mapping hardware for volume rendering would most likely find that the vast majority of them view limited texture memory as one of the most serious drawbacks of an otherwise fine technology. In this paper, we propose a compression scheme for static and time-varying volumetric data sets based on vector quantization that allows us to circumvent this limitation. We describe a hierarchical quantization scheme that is based on a multiresolution c ...

Keywords: Volume Rendering, Vector Quantization, Texture Compression, Graphics Hardware

14 Data integration and sharing II: Scientific data repositories: designing for a moving target



Etzard Stolte, Christoph von Praun, Gustavo Alonso, Thomas Gross

June 2003 **Proceedings of the 2003 ACM SIGMOD international conference on Management of data**

Publisher: ACM Press

Full text available: [pdf\(739.27 KB\)](#) Additional Information: [full citation](#), [abstract](#), [references](#), [citations](#), [index terms](#)

Managing scientific data warehouses requires constant adaptations to cope with changes in processing algorithms, computing environments, database schemas, and usage patterns. We have faced this challenge in the RHESSI Experimental Data Center (HEDC), a datacenter for the RHESSI NASA spacecraft. In this paper we describe our experience in developing HEDC and discuss in detail the design choices made. To successfully accommodate typical adaptations encountered in scientific data management systems ...

15 Database session 2: querying high-dimensional data II: Dimensionality reduction using magnitude and shape approximations



Ümit Y. Ogras, Hakan Ferhatosmanoglu

November 2003 **Proceedings of the twelfth international conference on Information and knowledge management**

Publisher: ACM Press

Full text available: [pdf\(193.50 KB\)](#) Additional Information: [full citation](#), [abstract](#), [references](#), [index terms](#)

High dimensional data sets are encountered in many modern database applications. The usual approach is to construct a summary of the data set through a lossy compression technique, and use this lower dimensional synopsis to provide fast, approximate answers to the queries. In this paper, we develop a novel dimensionality reduction technique based on partitioning the high dimensional vector space into orthogonal subspaces. First, we find a relation between the Euclidian distance of two n-dimensio ...

Keywords: high dimensional data, shape approximation, similarity search

16 A common data management infrastructure for adaptive algorithms for PDE solutions



Manish Parashar, James C. Browne, Carter Edwards, Kenneth Klimkowski

November 1997 **Proceedings of the 1997 ACM/IEEE conference on Supercomputing (CDROM)**

Publisher: ACM Press

Full text available: [pdf\(160.93 KB\)](#) Additional Information: [full citation](#), [abstract](#), [references](#), [citations](#)

This paper presents the design, development and application of a computational infrastructure to support the implementation of parallel adaptive algorithms for the solution of sets of partial differential equations. The infrastructure is separated into multiple layers of abstraction. This paper is primarily concerned with the two lowest layers of this infrastructure: a layer which defines and implements dynamic distributed arrays (DDA), and a layer in which several dynamic data and programming ab ...

Keywords: HP-adaptive finite elements, adaptive mesh-refinement, distributed dynamic data structures, fast multipole methods, parallel adaptive algorithm, problem solving environment

17 Hardware: Hardware-accelerated parallel non-photorealistic volume rendering



Eric B. Lum, Kwan-Liu Ma

June 2002 **Proceedings of the 2nd international symposium on Non-photorealistic animation and rendering**

Publisher: ACM Press

Full text available: [pdf\(12.03 MB\)](#) Additional Information: [full citation](#), [abstract](#), [references](#), [citations](#), [index terms](#)

Non-photorealistic rendering can be used to illustrate subtle spatial relationships that might not be visible with more realistic rendering techniques. We present a parallel hardware-accelerated rendering technique, making extensive use of multi-texturing and paletted textures, for the interactive non-photorealistic visualization of scalar volume data. With this technique, we can render a 512x512x512 volume using non-photorealistic

techniques that include tone-shading, silhouettes, gradient-base ...

Keywords: interactive visualization, non-photorealistic rendering, parallel rendering, scientific visualization, silhouette, texture graphics hardware, visual perception, volume rendering

18 Research track papers: IDR/QR: an incremental dimension reduction algorithm via QR decomposition

Jieping Ye, Qi Li, Hui Xiong, Haesun Park, Ravi Janardan, Vipin Kumar
August 2004 **Proceedings of the tenth ACM SIGKDD international conference on Knowledge discovery and data mining KDD '04**

Publisher: ACM Press

Full text available:  pdf(209.30 KB) Additional Information: [full citation](#), [abstract](#), [references](#), [index terms](#)


Dimension reduction is critical for many database and data mining applications, such as efficient storage and retrieval of high-dimensional data. In the literature, a well-known dimension reduction scheme is Linear Discriminant Analysis (LDA). The common aspect of previously proposed LDA based algorithms is the use of Singular Value Decomposition (SVD). Due to the difficulty of designing an incremental solution for the eigenvalue problem on the product of scatter matrices in LDA, there is little ...

Keywords: QR decomposition, dimension reduction, incremental learning, linear discriminant analysis

19 Articles: Data analysis and mining in the life sciences

Nam Huyn
September 2001 **ACM SIGMOD Record**, Volume 30 Issue 3

Publisher: ACM Press

Full text available:  pdf(1.00 MB) Additional Information: [full citation](#), [abstract](#), [references](#), [citations](#), [index terms](#)

Biotech companies routinely generate vast amounts of biological measurement data that must be analyzed rapidly and mined for diagnostic, prognostic, or drug evaluation purposes. While these data analysis tasks are critical to their success, they have not benefited from recent advances that emerged from database and KDD research. In this paper, we focus on two such tasks: on-line analysis of clinical study data, and mining broad datasets for biomarkers. We examine the new requirements that are no ...

20 Risk analysis: Simulation methodology for collateralized debt and real options: simulation methods for risk analysis of collateralized debt obligations

William J. Morokoff
December 2003 **Proceedings of the 35th conference on Winter simulation: driving innovation**

Publisher: Winter Simulation Conference

Full text available:  pdf(411.42 KB) Additional Information: [full citation](#), [abstract](#), [references](#)

Collateralized Debt Obligations (CDOs) are sophisticated financial products that offer a range of investments, known as tranches, at varying risk levels backed by a collateral pool typically consisting of corporate debt (bonds, loans, default swaps, etc.). The analysis of the risk-return properties of CDO tranches is complicated by the highly nonlinear and time dependent relationship between the cash flows to the tranche and the underlying collateral performance. This paper describes a multip ...

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